Calculation of exchange integrals in transition metals oxides using the LDA+U approach

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Theoretical determination of effective exchange coupling constants between the magnetic ions in transition metal oxides is a general and long standing problem. We propose a solution to the problem based on the mapping of the energy of noncollinear spin-spiral states calculated with the LDA+U method to the mean-field solutions of the effective spin Hamiltonian. The approach is applied to $Sr_2CuO_2Cl_2$, which can be described with good accuracy by a 2D Heisenberg model with only nearest-neighbor exchange, and to $Ba_2Cu_3O_4Cl_2$, which has two coupled anti-ferromagnetic spin systems. The same method is also used to determine the exchange constants between V^{4+} spins in the charge ordered low temperature phase of NaV_2O_5 and their dependence on the assumed kind of the charge ordering. The sensitivity of the calculated exchange constants to the strength of the on-site Coulomb repulsion U is analyzed.